ECOsystem Spaceborne Thermal Radiometer Experiment on Space Station (ECOSTRESS) Mission

Level 4 Water Use Efficiency Priestley-Taylor Jet Propulsion Laboratory (PT-JPL) Data User Guide

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2.0 Introduction

2.1 Purpose and Scope

This document is the Data User Guide for the Level 4 data product for the ECOsystem Spaceborne Thermal Radiometer Experiment on Space Station (ECOSTRESS) project. The Level 4 (L4) PT-JPL product provides evapotranspiration (ET) produced according to the PT-JPL algorithm described in the L4 Algorithm Theoretical Basis Document (ATBD) (JPL D-94645). This document applies to the Level 4 PT-JPL ESI product based upon data acquired by the ECOSTRESS radiometer instrument and will continued to be updated as needed. The purpose of this Data User Guide is to describe the ECOSTRESS end-user L4 data products and provide a guide for their use and interpretation.

2.2 Mission Overview

The ECOSTRESS instrument measures the temperature of plants and uses that information to better understand how much water plants use and how they respond to stress.

ECOSTRESS addresses three overarching science questions:

- How is the terrestrial biosphere responding to changes in water availability?
- How do changes in diurnal vegetation water stress impact the global carbon cycle?
- Can agricultural vulnerability be reduced through advanced monitoring of agricultural water consumptive use and improved drought estimation?

The ECOSTRESS mission answers these questions by accurately measuring the temperature of plants. Plants regulate their temperature by releasing water through pores on their leaves called stomata. If they have sufficient water, they can maintain their temperature. However, if there is insufficient water, their temperatures rise. This temperature rise can be measured with a sensor in space. ECOSTRESS uses a multispectral thermal infrared (TIR) radiometer to measure the surface temperature, deployed on the International Space Station. The instrument measures radiances at 5 spectral bands in the 8-12.5 μ m range with approximately 70 by 70 meter of spatial resolution on the ground.

On September 29th 2018, ECOSTRESS experienced an anomaly with its primary mass storage unit (MSU). ECOSTRESS has a primary and secondary MSU (A and B). On December 5th, the instrument was switched to the secondary MSU and operations resumed with initial acquisitions over Australia and wider coverage resumed on January 9th 2019. The initial anomaly was attributed to exposure to high radiation regions, primarily over the Southern Atlantic Anomaly, and the acquisition strategy was revised to exclude these regions from future acquisitions. On March 14th 2019, the secondary MSU experienced an anomaly, and acquisitions are temporarily on hold. Work is underway to implement a direct streaming option, which will bypass the need for mass storage units. The streaming acquisition mode will change the format of the data being collected. Specifically, the new collection mode will eliminate the 1.6 μ m (SWIR), 8.2 μ m (TIR), and 9.0 μ m (TIR) bands. To simplify product formats, the L1 and L2 products will continue to contain the datasets for these bands, but the datasets will contain fill values. This will be seen in products generated after May 15th 2019, when the instrument resumes operations. These changes are described in the detailed product specifications.

2.3 Applicable and Reference Documents

"Applicable" documents levy requirements on the areas addressed in this document. "Reference" documents are identified in the text of this document only to provide additional information to readers. Unless stated otherwise, the document revision level is Initial Release. Document dates are not listed, as they are redundant with the revision level.

2.3.1 Applicable Documents

ECOSTRESS Project Level 3 Science Data System Requirements (JPL D-94088).

ECOSTRESS Science Data Management Plan (JPL D-94607)

423-ICD-005 ICD Between ECOSTRESS SDS and LPDAAC

ECOSTRESS Level 1 Algorithm Theoretical Basis Documents (JPL D-94641, D-94642)

ECOSTRESS Level 1 Algorithm Specification Document

ECOSTRESS Level 2 Algorithm Theoretical Basis Documents (JPL D-94643, D-94644)

ECOSTRESS Level 2 Algorithm Specification Document

ECOSTRESS Level 3 (ET_PT-JPL) Algorithm Theoretical Basis Document (JPL D-94645)

ECOSTRESS Level 3 (ET_PT-JPL) Product Specification Document (JPL D-94636)

ECOSTRESS Level 3 (ET_PT-JPL) Algorithm Specification Document (JPL D-96970)

2.3.2 Reference Documents

2.4 ECOSTRESS Data Products

The ECOSTRESS mission will generate 13 different distributable data products (Reference Table below). The products represent four levels of data processing, with data granules defined as an image scene. Each image scene consists of 44 scans of the instrument mirror, each scan taking approximately 1.181 seconds, and each image scene taking approximately 52 seconds. Each image scene starts at the beginning of the first target area encountered during each orbit. Each orbit is defined as the equatorial crossing of an ascending International Space Stations (ISS) orbit.

ECOSTRESS Level 0 data include spacecraft packets that have been pre-processed by the Ground Data System (GDS). Level 1 products include spacecraft engineering data, the time-tagged raw sensor pixels appended with their radiometric calibration coefficients, the black body pixels used to generate the calibration coefficients, geolocated and radiometrically calibrated atsensor radiances of each image pixel, the geolocation tags of each pixel, and the corrected spacecraft attitude data. Level 2 products include the land surface temperature and emissivities of each spectral band retrieved from the at-sensor radiance data, and a cloud mask. Level 2 products also appear in image scene granules. Level 3 products contain evapotranspiration data derived from Level 2 data. Level 4 products contain evaporative stress index and water use efficiency derived from Level 3 data.

The ECOSTRESS products are listed in Table 1-1. This document will discuss only the Level 3 ET_PT-JPL product.

Product type	Description	
L0	Level 0 "raw" spacecraft packets	
L1A_ENG	Spacecraft and instrument engineering data, including blackbody gradient	
	coefficients	
L1A_RAW_ATT	Uncorrected spacecraft ephemeris and attitude data	
L1A_PIX	Raw pixel data with appended calibration coefficients	
L1B_GEO	Geolocation tags, sun angles, and look angles, and calibrated, resampled at-	
	sensor radiances	
L1B_ATT	Corrected spacecraft ephemeris and attitude data	
L2_LSTE	Land Surface temperature and emissivity	
L2_CLOUD	Cloud mask	
L3_ET_PT-JPL	Evapotranspiration retrieved from L2_LSTE using the PT-JPL Algorithm	
L3_ET_ALEXI	Evapotranspiration generated using the ALEXI/DisALEXI Algorithm	
L4_ESI_PT-JPL	Evaporative Stress Index generated with PT-JPL	
L4_ESI_ALEXI	Evaporative Stress Index generated with ALEXI/DisALEXI	
L4_WUE	Water Use efficiency	
L3 L4 QA	Quality Assessment fields for all ancillary data used in L3 and L4 products	

Table 1-1: ECOSTRESS Distributable Standard Products

3.0 ALGORITHM AND DATA DESCRIPTION

3.1 The Level 4 role in the ECOSTRESS data system

The ECOSTRESS Level 4 process requires the Level 2 data products for surface temperature and emissivity as well as the Level 1 geolocation information, and a significant number of ancillary data products from other sources (see section 2.2.3). The L3 ET product itself is used for creating the L4 products, Evaporative Stress Index (ESI) and Water Use Efficiency (WUE).

3.2 Input data sets

3.2.1 Requirements on inputs

All input data for the L4 product must be geolocated and time-ordered, and therefore have latitude, longitude, and time associated with each pixel. We do not pose strict requirements on the input products regarding format, projection, and spatio- temporal range. Given the wide range of sources of input data (presented in section x), the fetch and reprojection pipeline described in section x is designed to take care of processing this input data into formats, projections, and subsets as required by the application code described in section x.

3.2.2 ECOSTRESS input products

ECOSTRESS input data products used for the L4 data product are:

- Level 1B Geolocation
- Level 2 Land surface temperature
- Level 2 Surface emissivity
- Level 2 Cloud Mask

3.2.3 Ancillary input products

Other ancillary input data products used for the L4 data product are:

- MODIS Land
- MODIS Atmosphere
- Landsat 8
- NCEP

See the table below for more detailed information.

Table 2-1: L4 ET (PT-JPL) Ancillary Input Products

Product	Description	Provider
MOD04_L2	MODIS/Terra Aerosol	LAADS
MOD06_L2	MODIS/Terra Cloud	LAADS
MOD07_L2	MODIS/Terra Atmospheric Profile	LAADS
L8B10	Landsat 8 Band 10 Thermal 10.6-11.19 microns AWS	
L8B11	Landsat 8 Band 11 Thermal 11.5-12.51 microns	AWS
L8B2	Landsat 8 Band 2 Blue 450-510nm	AWS
L8B3	Landsat 8 Band 3 Green 530-590nm	AWS
L8B4	Landsat 8 Band 4 Red 640-670nm	AWS
L8B5	Landsat 8 Band 5 NIR 850-880nm	AWS
L8B6	Landsat 8 Band 6 SWIR 1570-1650nm	AWS
L8BQA	Landsat 8 Quality Flags	AWS
L8MTL	Landsat 8 Metadata	AWS
air.sig995	Air Temperature at Near-Surface Sigma .995	NCEP
rhum.sig995	Relative Humidity at Near-Surface Sigma .995	NCEP
tmin.2m.gauss	Minimum Temperature at 2m	NCEP
uwnd.sig995	U-Wind at Near-Surface Sigma .995	NCEP
vwnd.sig995	V-Wind at Near-Surface Sigma .995	NCEP
MCD12Q1	Land Cover Type Yearly L3 Global 500 m SIN Grid	LP-DAAC
MCD43A2	BRDF-Albedo Quality 16-Day L3 Global 500m	LP-DAAC
MCD43A3	Albedo 16-Day L3 Global 500m	LP-DAAC
MOD13Q1	Vegetation Indices 16-Day L3 Global 250m LP-DAAC	
MOD15A2H	MODIS FPAR and LAI 8-Day L4 Global 500m LP-DAAC	
MOD44W	MODIS 250m Water Mask	LP-DAAC

3.3 Output data sets

3.3.1 Attributes of output products

The ECOSTRESS Level 4 ESI output product fields are described in the table below:

Table 2-2: L4_WUE Product Data Definitions

Field Name	Type	Unit	Field Data
Group	Water Use Efficiency (per pixel, 5400 * 5632)		
WUEavg	Float32	GPP/ET	Water Use Efficiency

Unlike the instantaneous L3 PT-JPL and L4 ESI products, the L4 WUE product is calculated at a daily timestep. Water Use Efficiency (WUEavg) is the ratio of carbon stored by plants to water evaporated by plants. This ratio is given as grams of carbon stored per kilogram of water evaporated over the course of the day from sunrise to sunset on the day when the ECOSTRESS granule was acquired.

4.0 SOFTWARE DESIGN

4.1 Overview

The ECOSTRESS pipeline prepares source data from a multitude of remote sensing and reanalysis data products. These source data are retrieved, preprocessed, and resampled to an ECOSTRESS scene. These preprocessed data are run through a series of models to produce the ECOSTRESS product.

4.2 Description of major code sections

4.2.1 Pre-processing pipeline



The downloader PGE begins by calculating which source data granules spatio-temporally intersect the given ECOSTRESS scene. A polygon surrounding the convex hull of latitude/longitude pairs contained in the L1B geolocation arrays is taken as the destination region. Source regions from Landsat 8 in terms of Landsat path/row are determined by intersecting the target ECOSTRESS polygon with the static set of polygons in the WRS2-Descending region extent system. A static set of polygons in the MODIS Sinusoidal Grid are also intersected against the target footprint of the ECOSTRESS scene to select the horizontal and vertical index pairs for MODIS land products.

Selection of swath granules for the MODIS atmospheric products requires knowledge of the Terra satellite's orbit. To calculate the orbit of Terra, the Two-Line Element (TLE) observed by the Air Force at the time of ECOSTRESS overpass is queried from *spacetrack.com*. This TLE is

used to calculate the swath ground track of Terra in a 12-hour radius surrounding the ECOSTRESS overpass time using the *pyephem* library. The boundary of potentially matching MODIS swath granules is calculated by dividing Terra's swath ground track into 5-minute increments beginning at UTC midnight and applying a constant cross-track swath width. The polygons surrounding these temporally intersecting MODIS swaths are then intersected against the target ECOSTRESS polygon to determine the set of MODIS swath granules that should be retrieved.

With the required granules of source data known, remote servers are crawled to resolve these granules to URLs of available granules for retrieval. Source Landsat 8 files are addressed on Amazon Web Services as individual GeoTIFF files for each band. Addresses for MODIS land data are queried from the Land Processes Distributed Active Archive Center (LP-DAAC) Inventory API. Addressed for MODIS atmosphere granules are obtained by crawling the CSV listings of the Level-1 and Atmosphere Archive & Distribution System Distributed Active Archive Center (LAADS DAAC) HTTP Interface.

With the addresses of required granules recorded, the downloader PGE makes calls to WGET to retrieve these files from the remote servers, organized into a consistent directory structure on the local filesystem. In order to conserve on storage requirements, all runs of the ECOSTRESS downloader retrieve to a collective local mirror. WGET is able to efficiently retrieve only files that it has not already retrieved.

The preprocessor PGE loads and preprocesses the retrieved source data granules. Both Landsat and MODIS record their datasets in 16-bit integer analogs to floating point values. These Digital Numbers (DNs) in the Landsat bands are converted to reflectance using linear parameters read from the Landsat metadata, and these reflectance values are used to calculate NDVI and albedo. Atmospheric and land inputs are ready-made as products in MODIS but are also linearly converted into real units and filtered by accompanying quality flags.

With source data preprocessed at their original locations, these data are ready to be projected onto the target ECOSTRESS scene. Since it is only possible to project between gridded surfaces, intermediate gridded surfaces must be created to represent the source MODIS swaths and destination ECOSTRESS swath. The *pyresample* library is used to resample by nearest neighbor between swaths and their representative grids. The *rasterio* library is used to warp data between gridded surfaces, smoothed by cubic interpolation. These techniques are combined to mosaic preprocessed source data over the extent of the ECOSTRESS scene and resample this mosaic onto the ECOSTRESS geolocation provided by the L1B product. Finally, these data are stored as the inputs for the PT-JPL and disALEXI PGEs.

This data-store of model forcings passed to the model PGEs is organized by variable and date into a directory structure and written in Hierarchical Dataset Format (HDF5) using the *h5py* library. HDF5 was chosen as an intermediate file format to accommodate geolocated/non-gridded data.

4.2.2 Computation of evapotranspiration



The PT-JPL PGE loads the preprocessed forcing data prepared by the preprocessor PGE and runs them through a sequence of surface energy balance models. All variables, including geolocation, are loaded from the forcing data store created by the preprocessor using the HDF5 library. The Forest Light Environmental Simulator (FLiES) calculates incoming shortwave radiation from atmospheric observations. This is accomplished by querying a multidimensional array of precomputed FLiES model output as a lookup table. The Breathing Earth Systems Simulator (BESS) ingests the ECOSTRESS LST as outgoing longwave radiation. This balance is closed to produce net radiation, the total energy available at the surface. The Priestley-Taylor Jet Propulsion Laboratory (PT-JPL) model calculates transpiration, interception, and soil evaporation from net radiation using the Priestley-Taylor formula constrained by observed land surface properties. These partitions and their total are written to the ECOSTRESS product file using the HDF5 library.

5.0 OTHER CONSIDERATIONS

5.1 Error handling

Error handling is managed using Python's exception handling framework. Exception classes were designed for all foreseeable disruptions to data processing, each of which is assigned a unique exit code that is returned to the Process Control System (PCS).

5.2 Dependencies on existing software

The Anaconda distribution of Python 3.5 was chosen as the platform for the downloader/preprocessor subsystem because of its good support for geospatial data processing. The conda environment manager included in Anaconda provides seamless dependency management for the scientific, geospatial, and data management packages required for ECOSTRESS. These package dependencies include: pandas, affine, ephem, fiona, geopandas, h5py, lxml, netcdf4, nose, numpy, pyproj, python-dateutil, rasterio, requests, shapely, six, spacetrack, bs4, usgs, homura, termcolor, geocoder, scipy, pyresample, future, pygments, xmltodict, scikit-image, jsonmerge, rasterstats, and untangle.

The C++ language was chosen to implement the PT-JPL model code to maximize the efficiency of processing large arrays. The main dependency linked to by the PT-JPL PGE is the Hierarchical Data Format (HDF) library, which is required for writing the ECOSTRESS product to file.

5.3 Assumptions and limitations

This software assumes daytime acquisition. It is designed not to run for granules acquired at night. This software also assumes precise (< 50 m) geolocation. ECOSTRESS granules that could not be precisely geolocated in the L1B GEO product are not processed into the L4 PT-JPL product. These procedures are in place to ensure that only high-quality raster data are produced in the L4 product, but results in about 1/7 of available ECOSTRESS scenes processing into PT-JPL.

This software also assumes clear-sky conditions. The cloud mask produced in the L2 LSTE product is applied to the L4 product. All pixels considered to be cloud or adjacent to clouds are represented as blank pixels by the IEEE 754 NaN value. This may result in L4 PT-JPL scenes in which a large portion or the entirety of the scene is blank.

5.4 Quality assessment and recording

No original quality flags are produced. Instead the quality flags of the source data products are resampled by nearest neighbor onto the geolocation of the ECOSTRESS scene. A quality flag array for each input dataset, when available, is collected into a combined QA product accompanying the PT-JPL product file.

6.0 APPENDIX A: ABBREVIATIONS AND ACRONYMS

ALEXI Atmospheric-Land Exchange Inversion
ASD Algorithm Specifications Document
ATBD Algorithm Theoretical Basis Document
BESS Breathing Earth Systems Simulator
DAAC Distributed Active Archive Center
DisALEXI ALEXI Disaggregation algorithm

ECOSTRESS ECOsystem Spaceborne Thermal Radiometer on Space Station

ESI Evaporative Stress Index ET Evapotranspiration

FLiES Forest Light Environmental Simulator

GDS Ground Data System
HDF Hierarchical Data Format

Hz Hertz

ICD Interface Control Document
ISS International Space Station
JPL Jet Propulsion Laboratory

Km kilometer

L0 – L4 Level 0 through Level 4

LP Land Processes

LST Land Surface Temperature

LSTE Land Surface Temperature and Emissivity

m meter

MODIS Moderate Resolution Imaging Spectroradiometer NASA National Aeronautics and Space Administration NCEP National Centers for Environmental Protection

netCDF Network Common Data Format

PCS Process Control System

PGE Product Generation Executable
PSD Product Specifications Document

PT-JPL Priestley-Taylor-JPL QA Quality Assurance

SDOS Science Data Operations System

SDS Science Data System
TBD To Be Determined
TBR To Be Reconciled
TBS To Be Specified

USDA United State Department of Agriculture

USGS United States Geological Society UTC Coordinated Universal Time

WUE Water Use Efficiency

XML Extensible Markup Language

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